Self–Similar Crossover in Statistical Physics

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Abstract

An analytical method is advanced for constructing interpolation formulae for complicated problems of statistical mechanics, in which just a few terms of asymptotic expansions are available. The method is based on the self–similar approximation theory, being its variant where control functions are defined from asymptotic crossover conditions. Several examples from statistical physics demonstrate that the suggested method results in rather simple and surprisingly accurate formulae.

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1   Introduction

In many problems of statistical physics one encounters the so–called crossover phenomena, when a physical quantity qualitatively changes its behaviour in different domains of its variable. To be more precise, we may specify a crossover as follows. Let a function $f(x)$ represent a physical quantity of interest, with a variable running through the interval $x_1 \leq x \leq x_2$. And let the behaviour of this function, describing some physical process, be essentially different near the boundary points x_1 and x_2. Assume that the function varies continuously from $f(x_1)$ to $f(x_2)$, as x changes from x_1 to x_2. Then we may say that the function in the interval $[x_1, x_2]$ undergoes a crossover between $f(x_1)$ and $f(x_2)$.

Crossover behaviour of different physical quantities is so ubiquitous in nature that one could list a plenty of examples. For instance, a number of physical quantities essentially change their behaviour when passing from the weak–coupling to strong–coupling limit [1]. In the theoretical description of crossover there exists a problem which is common for practically all physical applications. Real physical systems are usually so complicated that describing them equations almost never can be solved exactly. However, it is often possible to find asymptotic expansions of solutions in vicinity of boundary points. The natural arising problem is how to construct an accurate approximation for the sought function, valid on the whole domain of its variable, knowing only its asymptotic behavior near the boundaries. This problem is aggravated by the fact that only a few terms of the asymptotic expansions are usually available. In such a case the problem looks unsolvable.

The most known method of treating the interpolation problem is by using the so–called two–point Padé approximants [2-4] or, equivalent to the latter, the Thron continued fractions [5,6]. In many cases the two–point Padé approximation yields quite reasonable interpolation formulas. However, the usage of this method has not become widespread because of the following shortcomings of the Padé approximants:

(i) When constructing these approximants, one often obtains spurious poles yield-

ing unphysical singularities [2-4]. A sequence of Padé approximants may even have infinitely many poles [7].

(ii) A number of examples are known when Padé approximants are not able to sum perturbation series even for small values of an expansion parameter [8,9].

(iii) In the majority of cases, except some trivial examples, to reach a reasonable accuracy, one needs to have tens of terms in perturbative expansions [4]. While, as is emphasized above, in physically interesting problems one often has only a few terms.

(iv) Defining the two–point Padé approximants one always confronts the ambiguity in distributing the coefficients, that is, in deciding which of the coefficients must reproduce the left–side expansion and which the right–side series [1-6]. Such an ambiguity increases with the increase of approximants orders, making it difficult to compose two–point Padé tables. And for the case of a few terms, this ambiguity makes the two–point Padé approximants practically unapplicable. A nice analysis of the latter difficulty was done in Ref. [10], where it was shown that, for the same problem, one may construct different two–point Padé approximants all having correct left–side and right–side limits, but differing from each other in the intermediate region by a factor of 40 which gives 1000% of uncertainty. This clearly demonstrates that in the case of short series the two–point Padé approximation not only cannot provide a reasonable quantitative approach but even does not permit to get a qualitative description. The latter concerns the general situation, although there can happen some trivial cases when two–point approximants make sense even being built with a few perturbative terms. However, their application to such few–term cases, in general, is absolutely unreliable.

(v) The two–point Padé approximants can be used for interpolating between two different expansions not always, but only when these two expansions have compatible variables [2-4,9]. When these expansions have incompatible variables, the two–point Padé approximants cannot be defined in principle.

(vi) When interpolating between two points, one of which is finite and another is

at infinity, one is able to describe at infinity only rational powers [2-4]. The impossibility to deal with nonrational powers limits the applicability of the two–point Padé approximation.

(vii) The problem of approximating the functions increasing at infinity is especially difficult. A two–point Padé approximant can treat only a power–law increase [1-5] and is not able to describe other types of behaviour. But in physical problems the functions of interest often exhibit at infinity quite different behaviour, for example, growing exponentially or following other more complicated ways. In such cases the two–point Padé approximants are useless.

The difficulties listed above are well known and discussed in literature. We have cited here only some important references [1-10]. More details on mathematical problems in Padé approximation and its applications can be found in several volumes of papers, e.g. in Ref. [11].

As follows from the above discussion, the two–point Padé approximation in many cases is not applicable. It is evident that there is a necessity of developing a more general approach which could overcome the discussed difficulties and would be applicable to a larger variety of problems, including those for which the two–point Padé approximants cannot be used. It is important that such an approach would provide relatively simple analytical formulas for the physical quantities of interest. The advantage of having analytical expressions, as compared to just numbers that could be obtained from a numerical procedure, is in the convenience of analysing such expressions with respect to various parameters entering into them. Therefore, we keep in mind an analytical, rather than numerical, method that would combine relatively simple representations for physical quantities with their good accuracy.

It is worth emphasizing that to derive a new physical formula, valid in the whole range of physical variables, is not merely a mathematical challenge but this provides new physics, since in the majority of cases realistic physical problems correspond neither to weak coupling regime nor to strong coupling limit, but to the intermediate

range of parameters. Therefore, it is of great importance for physics to possess a general mathematical tool permitting to derive explicit crossover formulas for arbitrary physical phenomena.

In the present paper we suggest an approach for treating this problem. Our approach is based on the self–similar approximation theory [12-22] permitting an accurate reconstruction of functions from a few terms of perturbative expansions. The effectiveness of the self–similar approximation theory is due to the usage of powerful techniques of dynamical theory and optimal control theory. Fast convergence of renormalized sequences is achieved by means of control functions. In the algebraic self-similar renormalization [20-22], we required the algebraic invariance of renormalization-group flow. Then, control functions are introduced as powers of a multiplicative algebraic transformation. These control functions are defined by the stability and fixed-point conditions for a dynamical system called the approximation cascade. In general, the evolution equations for a dynamical system can be completed by additional constraints whose existence imposes restrictions on the definition of control functions.

Crossover problem presents an example when additional constraints appear absolutely naturally. Really, assume that we have a k-order expansion $p_k(x)$ approximating the sought function $f(x)$ in the asymptotic vicinity of the left boundary $x = x_1$. And suppose that we are given an asymptotic behavior of this function near the right boundary $x = x_2$. For a moment, take for simplicity that we are given the value $f(x_2)$ at the right boundary point $x = x_2$. When constructing a self-similar approximation $f_k^*(x)$ by renormalizing the left boundary expansion $p_k(x)$, we have as an additional constraint the right boundary condition $f_k^*(x_2) = f(x_2)$.

We show below that the algebraic self-similar renormalization provides a very convenient tool for treating the crossover problem. This approach permits us to find, having just a minimal information about the asymptotic behavior of a function near boundary points, a quite accurate approximation for the whole region of the variable. In the majority of cases the maximal error of a self–similar approximation is a few percent and in many cases not more than one percent. In addition to being quite accurate,

this approximation is usually given by very simple expressions that are easy to analyze. We illustrate the approach by several examples from different branches of statistical physics. The variety of considered cases emphasizes the generality of the approach and proves that it is a very effective tool for treating arbitrary crossover phenomena.

Recently, we have applied such an interpolation approach to several quantum–mechanical problems [23]. However, what makes the latter principally different from the problems of statistical physics is that in quantum mechanics one usually possesses quite a number of terms of perturbative expansions, while in statistical physics this luxury is rather rare, so that in the majority of cases one is able to derive just a few perturbative terms. In the present paper we aim at showing that our interpolation method does work for those complicated problems of statistical physics where only a few terms of asymptotic expansions are available and other methods are not applicable. Nevertheless, the self–similar interpolation makes it possible to treat even such complicated crossover problems, obtaining simple and accurate formulae.

2   General approach

In this section, we formulate the general scheme of the approach not specifying the physical nature of a considered function. Let us be interested in a function $f(x)$ of a real variable x. Assume that in the vicinity of some point $x = x_0$ there exist asymptotic expansions $p_k(x, x_0)$, with $k = 0, 1, 2, \ldots$, corresponding to this function,

$$f(x) \simeq p_k\ (x, x_0), \qquad x \to x_0 \ . \tag{1}$$

Following the algebraic self–similar renormalization procedure [20-22], we define the algebraic transform

$$P_k(x, s, x_0) = x^s p_k(x, x_0) \ , \tag{2}$$

where s is yet unknown, and later will play the role of a control function. The transform inverse to that in Eq.(2) is

$$p_k(x, x_0) = x^{-s} P_k(x, s, x_0) \ . \tag{3}$$

Then we have to construct an approximation cascade with a trajectory bijective to the approximation sequence $\{P_k\}$. This procedure with all necessary mathematical foundations and details has been described in Refs. [13-19]. So, we sketch here only the main steps needed for grasping the idea of the method and we concentrate on those formulas that permit us to apply the method for crossover phenomena.

Define an expansion function $x = x(\varphi, s, x_0)$ by the equation

$$P_0(x, s, x_0) = \varphi, \qquad x = x(\varphi, s, x_0) \,, \tag{4}$$

where P_0 is the first available term from the sequence $\{P_k\}$. Introduce a function

$$y_k(\varphi, s, x_0) = P_k(x(\varphi, s, x_0), s, x_0) \,. \tag{5}$$

The transformation inverse to Eq. (5) reads

$$P_k(x, s, x_0) = y_k(P_0(x, s, x_0), s, x_0) \,. \tag{6}$$

The family of endomorphisms, $\{y_k\}$, forms a cascade with the velocity field

$$v_k(\varphi, s, x_0) = y_{k+1}(\varphi, s, x_0) - y_k(\varphi, s, x_0) \,. \tag{7}$$

The trajectory of the cascade $\{y_k\}$ is, by definitions (5) and (6), bijective to the approximation sequence $\{P_k\}$. Embedding the approximation cascade into an approximation flow [16-19] and integrating the corresponding evolution equation, we come to the evolution integral

$$\int_{P_k}^{P_{k+1}^*} \frac{d\varphi}{v_k(\varphi, s, x_0)} = \tau \,, \tag{8}$$

in which $P_k = P_k(x, s, x_0)$ is any given term from the approximation sequence $\{P_k\}$; $P_{k+1}^* = P_{k+1}^*(x, s, \tau, x_0)$ is a self–similar approximation representing a fixed point of the approximation cascade; and τ is an effective minimal time necessary for reaching the fixed point.

Recall that we started with a sequence $\{p_k\}$ of asymptotic expansions for the considered function $f(x)$. Then we passed to the sequence $\{P_k\}$ by means of the algebraic

transformation (2). Now we have to return back employing the inverse transformation (3). To this end, we set

$$F_k^*(x, s, \tau, x_0) = x^{-s} P_k^*(x, s, \tau, x_0) \ . \tag{9}$$

The quantities s and τ are the control functions guarantying the stability of the method, that is, the convergence of the procedure. These functions are to be defined by the stability conditions, such as the minimum of multiplier moduli, together with additional constraints, like, e.g., boundary conditions. Let us find from such conditions $s = s_k$ and $\tau = \tau_k$. Substituting these into Eq.(9), we obtain the self–similar approximation

$$f_k^*(x, x_0) = F_k^*(x, s_k, \tau_k, x_0) \tag{10}$$

for the function $f(x)$. We retain here the notation for the point x_0 in order to show that the approximation (10) has been obtained by renormalizing $p_k(x, x_0)$ which, according to Eq. (1), is an asymptotic expansion of $f(x)$ in the vicinity of the point $x = x_0$.

Now assume that the variable x changes in the interval $x_1 \leq x \leq x_2$ and that the asymptotic behavior of a function $f(x)$ is known near the boundaries of this interval. The latter means that in Eq. (1) we have to put, instead of x_0, either x_1 or x_2. Let us take, for concreteness, the boundary points $x_1 = 0$ and $x_2 \to \infty$. Then we have two types of expansions, $p_k(x, 0)$ and $p_k(x, \infty)$. Following the procedure described above, we can construct, in the place of Eq. (9), two quantities, $F_k^*(x, s, \tau, 0)$ and $F_k^*(x, s, \tau, \infty)$.

As is discussed above, the control functions s and τ are to be defined from stability conditions plus additional constraints. The natural such constraints for the crossover problem can be formulated as follows. Suppose we have constructed the renormalized expression $F_k^*(x, s, \tau, 0)$ starting from the left asymptotic expansion $p_k(x, 0)$. By this construction, the function F_k^* has correct asymptotic behavior near the left boundary. But in order to correctly represent the sought function in the whole interval of $x \in [0, \infty)$, the renormalized expression F_k^* must have the correct asymptotic behavior when

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approaching the right limit. This implies the validity of the condition

$$\lim_{x \to \infty} |F_k^*(x, s, \tau, 0) - p_i(x, \infty)| = 0 , \tag{11}$$

imposing constraints on $s = s_k$ and $\tau = \tau_k$. We shall call Eq. (11) providing the correct crossover behavior from the left to the right boundary the *left crossover condition*. The quantity s_k can be called the *left crossover index,* and τ_k, the *left crossover time.* For the self–similar approximation (10) we get, in this way,

$$f_k^*(x, 0) = F_k^*(x, s_k, \tau_k, 0) , \tag{12}$$

which may be named the *left self–similar approximation*, or the *left crossover approximation.*

The analogous reasoning works, as is clear, when we are considering the crossover from the right to left. Then we obtain the *right crossover condition*

$$\lim_{x \to 0} |F_k^*(x, s, \tau, \infty) - p_j(x, 0)| = 0 , \tag{13}$$

imposing constraints on $s = s_k$ and $\tau = \tau_k$, thus defining the *right crossover index* s_k and the *right crossover time* τ_k. As a result, we come to the *right self–similar approximation*, or the *right crossover approximation*

$$f_k^*(x, \infty) = F_k^*(x, s_k, \tau_k, \infty) . \tag{14}$$

In general, from the left and the right approximations, (12) and, respectively, (14), we can compose the *average self–similar approximation*, or *average crossover approximation*

$$f_k^*(x) = \frac{1}{2} [f_k^*(x, 0) + f_k^*(x, \infty)] . \tag{15}$$

The suggested general approach to reconstructing crossover functions can be employed for any crossover phenomena. In particular applications, it can happen that we possess a reliable asymptotic expansion only from one side of the crossover domain, and from another side just one term is available. In this case, as is clear, we are not able to construct both left and right self-similar approximations, but only one of them.

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Nevertheless, such one–side approximations are usually quite accurate, as we show by examples in the following sections. The possibility of constructing accurate approximations, when we have a perturbative series only from one side of the crossover region and a sole asymptotic term from another side, is very important since this situation constantly occurs in realistic physical problems. We shall demonstrate in what follows how it is possible to improve the accuracy of such one–side approximations by combining the terms of a given one–side series and defining the crossover indices so that to satisfy the asymptotic limit from another side, in accordance with the crossover conditions (11) or (13).

In order to emphasize that the suggested approach does work even for the cases with a very scarce information about the sought function, let us consider a simple example. Suppose that we know the asymptotic behavior of a function near the left boundary, where $x \to 0$, only in the linear approximation

$$p_1(x, 0) \simeq a_0 + a_1 x , \qquad a_0, \ a_1 \neq 0 . \tag{16}$$

And assume that only one asymptotic term is known from the right side,

$$p_1(x, \infty) \simeq A \ x^n , \qquad A, \ n \neq 0 , \tag{17}$$

as $x \to \infty$. In such an extreme case of minimal information, it looks like there is no a regular way of recovering the function for the whole axis $0 \leq x < \infty$. However, our approach, based on the idea of self–similarity, permits us to recover the sought function.

Following the procedure described above, in the place of Eq.(9), starting from expansion (16), we obtain

$$F_1^*(x, s, \tau, 0) = a_0 \left(1 - \frac{a_1 \tau}{a_0 s} \ x \right)^{-s} . \tag{18}$$

With Eqs.(17) and (18), the left crossover condition (11) reads

$$\lim_{x \to \infty} \left| a_0 \left(1 - \frac{a_1 \tau}{a_0 s} \ x \right)^{-s} - A \ x^n \right| = 0 ,$$

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From here the left crossover index s_1 and the left crossover time τ_1 are uniquely defined as follows:

$$s_1 = -n \, , \qquad \tau_1 = n \frac{a_0}{a_1} \left(\frac{A}{a_0} \right)^{1/n} \, . \tag{19}$$

Substituting these values into Eq. (18), as is prescribed by Eq. (12), we recover the left crossover approximation

$$f_1^*(x,0) = a_0 \left[1 + \left(\frac{A}{a_0} \right)^{1/n} x \right]^n \, . \tag{20}$$

At large $x \to \infty$, expression (20) reduces to the limit (17). When $x \to 0$, then we have the linear behavior

$$f_1^*(x,0) \simeq a_0 + a_1^* x \, ,$$

where $a_1^* = n a_0 \left(A/a_0 \right)^{1/n}$ is the renormalized coefficient. Such a renormalization is typical of renormalization group techniques, as is discussed in Refs. [20-22].

Thus, even having so scanty information about the asymptotic properties of a function, as in the above example, our approach allows us to reconstruct, in a systematic way, the function for the whole domain of its variable. This reconstruction becomes possible owing to the idea of self–similarity which our approach is based on and due to the convenient introduction of control functions through the algebraic transformation. The idea of self–similarity, complimented by the property of algebraic invariance, eliminates the umbiguity typical of divergent series in the standard perturbative approaches. In the sections that follow, it will be shown that the accuracy of so constructed self-similar approximations is rather good.

Note that achieving good accuracy with a limited number of terms of an asymptotic expansion should not be treated as surprising. Asymptotic series are known to provide reasonable accuracy when up to some optimal number of terms are taken [24], the subsequent terms only spoil the picture being, in this sense, excessive. Whether there are such excessive terms or not is decided, in our approach, by stability and crossover conditions. As soon as these are satisfied, there are no excessive terms. And if adding more terms does not allow us to satisfy these conditions, the added terms are to be

considered excessive. Fortunately, the real life and realistic physical problems are so complicated that we practically never have excessive terms, but vice versa, have to deal with very short expansions containing only a few terms.

3   Zero–dimensional model

For illustrative purpose, we start with a simple model example. Consider the partition function of a zero-dimensional anharmonic model, represented by the integral

$$J(g) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp\left(-x^2 - gx^4\right) dx, \tag{21}$$

with the integrand possessing a single "vacuum" state, located at the point $x = 0$. The weak–coupling expansion of this integral in powers of the coupling parameter g, around the vacuum state, leads to divergent series,

$$J(g) \simeq a + bg + cg^2 + \dots , \qquad (g \to 0), \tag{22}$$

where

$$a = 1 , \qquad b = -\frac{3}{4} , \qquad c = \frac{105}{32} .$$

The so-called strong-coupling expansion, in inverse powers of the coupling constant, can be written down as well:

$$J(g) \simeq Ag^{-1/4} + Bg^{-3/4} + Cg^{-5/4} + \dots , \qquad (g \to \infty) , \tag{23}$$

with

$$A = \frac{1.813}{\sqrt{\pi}} , \qquad B = -\frac{0.612}{\sqrt{\pi}} , \qquad C = \frac{0.227}{\sqrt{\pi}} .$$

Following the approach of Section 2, one can derive the right crossover approximation,

$$J^*(g, \infty) = aA \left(A^2 + a^2 g^{1/2}\right)^{-1/2} , \tag{24}$$

with the right crossover index $s = 1/2$ and crossover time $\tau = -A^3/(2a^2 B) = 1.55$. At $g = 1$, the percentage error of formula (24), is equal to -7.38%, while the maximal error is reached at $g = 0.35$ and equals -7.96%.

The left crossover approximation is given as follows:

$$J^*(g, 0) = aA \left(A^4 + a^4 g \right)^{-1/4} , \tag{25}$$

with the left crossover index $s = 1/4$, and crossover time $\tau = -a^5/(4A^4 b) = 0.304$. At $g = 1$, the percentage error of Eq. (25) is 10.13%, while the maximal error at $g = 2.5$, is equal to 10.53%. We conclude, that the crossover approximations (24) and (25) may be viewed, correspondingly, as the lower and upper bounds for the integral (21). The average, defined by Eq. (15),

$$J^*(g) = \frac{J^*(g, 0) + J^*(g, \infty)}{2} ,$$

possesses the correct leading asymptotes and approximates the exact result at $g = 1$ with the percentage error of 1.37%. And the maximal error, at $g = 3$, is 2.21%.

4   Lattice gauge model

The vacuum energy density f_0 of the (3+1)–dimensional SU(2) lattice gauge model in its weak–coupling, asymptotically free regime, may be presented in the form of an expansion in powers of the parameter $x = 4/g^4$, where g stands for the coupling [25]:

$$f_0 \simeq Ax + B\sqrt{x} + \dots , \qquad (x \to \infty) , \tag{26}$$

where

$$A = -6, \qquad B = 7.1628 .$$

In its strong–coupling limit, f_0 can be presented as follows [25]:

$$f_0 \simeq ax^2 + bx^4 + \dots , \qquad (x \to 0) , \tag{27}$$

with

$$a = -1 , \qquad b = 0.03525 .$$

Because of the interfering roughening transition, the quality of the high–order terms in the strong–coupling expansion is doubtful [25], so we use only its leading terms. The

left crossover approximation can be readily written down as

$$f^*(x, 0) = ax^2 \left[1 + \left(\frac{a}{A} \right)^2 x^2 \right]^{-1/2} , \qquad (28)$$

where we have used

$$s = \frac{1}{2} , \qquad \tau = -\frac{a^3}{2bA^2} .$$

The numbers generated by formula (28), practically coincide in the region $x \in [0.1, 1.1]$ with estimates obtained in [25] from the strong–coupling approximants. The right crossover approximation can be obtained as well, but its accuracy is worse than that of Eq. (28).

5 One–dimensional Bose system

The ground–state energy of the one–dimensional Bose system with the δ–functional repulsive interaction potential is known in a numerical form from the Lieb–Liniger exact solution [26]. It is desirable, nevertheless, to have a compact analytical expression for the ground–state energy $e(g)$ as a function of the δ–function strength g, valid for arbitrary g. In the weak–coupling limit an exact analytical result is known:

$$e(g) \simeq g , \qquad (g \to 0) , \qquad (29)$$

obtained in Ref. [26], while in the strong–coupling limit another exact result, obtained by Girardeau [27], is available:

$$e(g) \simeq \frac{\pi^2}{3} , \qquad (g \to \infty) . \qquad (30)$$

The higher–order terms in these expansions were derived by approximate methods, the next term in the weak–coupling limit being $\approx bg^{3/2}$, and in the strong–coupling limit $\approx Bg^{-1}$. We shall not use the approximate values for the coefficients, b and B (see e.g. [13] and references therein), writing instead trial expansions and determining the coefficients by matching the two asymptotic forms for the ground state energy. Following

the standard approach of Section 2, we obtain the right crossover approximation:

$$e^*(g, \infty) = \frac{\pi^2}{3} g \left(g + \frac{\pi^2}{3} \right)^{-1},$$ (31)

with the right crossover index $s = 1$ and $B = (\pi^2/3)^2$. Although, Eq. (31) can be further simplified, we leave it in present form in order to stress the origin of its different parts. Simple expression (31) works with surprising accuracy of about $1 - 2\%$, up to $g \sim 10$, till there are numerical data available for comparison [26]. The left crossover–type expression can be written as well, following the standard procedure, but its accuracy is inferior to that of Eq. (31).

6   One–dimensional ferromagnet

Low–dimensional magnetic systems give a plenty of examples of the crossover phenomena, when only the asymptotic behavior with respect to different parameters, such as spin, temperature etc, is known and the intermediate region, in most of the cases, could be reached only numerically. The crossover self–similar approximations offer simple analytical expressions for the intermediate region. We put below, for simplicity, the exchange integral $J = 1$.

6.1   Zero–field thermodynamics

The free energy F and magnetic susceptibility χ of the one–dimensional Heisenberg ferromagnet of spin S, within the framework of the spin-wave approximation, valid at temperatures $T \to 0$, has the form of an expansion in powers of T [28]:

$$F \simeq a(S)T^{3/2} + b(S)T^2 + \dots, \qquad (T \to 0),$$ (32)

in which

$$a(S) = -\frac{\zeta(3/2)}{(2\pi)^{1/2}} \left(\frac{1}{2S} \right)^{1/2}, \qquad b(S) = \frac{1}{4S^2},$$

and

$$\chi \simeq A(S)T^{-2} + B(S)T^{3/2}, \qquad (T \to 0),$$ (33)

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where

$$A(S) = \frac{8}{3}S^4 , \qquad B(S) = -A(S)\frac{3\zeta(1/2)}{\sqrt{2\pi S}} .$$

As $T \to \infty$, a different asymptotic behavior happens [29]:

$$F \simeq -T \ln(1 + 2S) \qquad (T \to \infty) \tag{34}$$

and

$$\chi \simeq \frac{4S(S+1)}{3T} \qquad (T \to \infty). \tag{35}$$

Applying the standard approach of Section 2, we obtain for the free energy the following left crossover approximation, corresponding to the left crossover index $s = 1$,

$$F^*(T, S) = a(S)\frac{T^{3/2}}{1 - [b(S)/a(S)]\tau T^{1/2}} , \qquad \tau = \frac{a^2(S)}{b(S)\ln(1 + 2S)} , \tag{36}$$

and the expression for specific heat $C^* = -T d^2 F^*(T, S)/dT^2$ as

$$C^*(T, S) = -\frac{1}{4}T^{1/2}a^3(S)\frac{-3a(S) + b(S)\tau T^{1/2}}{[-a(S) + b(S)\tau T^{1/2}]^3} . \tag{37}$$

The position, height and spin–dependence of the maximum occurring in the expression for $C^*(T, S)$ are in qualitative agreement with numerical results for finite chains [30].

The left crossover approximation for the renormalized susceptibility is

$$\chi^* = \frac{A(S)}{T^2}\left[1 + \frac{B(S)}{2A(S)}\tau T^{1/2}\right]^2 , \qquad \tau = \frac{A(S)}{B(S)}\left[\frac{16S(1+S)}{3A(S)}\right]^{1/2} , \tag{38}$$

with the left crossover index $s = -2$. The expressions (36) and (38) are very accurate for $S = 1/2$, where they practically coincide with the results of a numerical solution of the thermodynamic Bethe–ansatz equations [28].

6.2   Spin waves at finite temperatures

Variational theory, as applied at low temperatures [31], gives the temperature–dependent expression for the spin–wave energy ω_k for $S = 1/2$ in the form

$$\omega_k = 2Z(T)\,|\sin(k)| , \qquad Z(T) \simeq \frac{1}{2}\pi\left[1 - \frac{2}{3}\left(\frac{T}{2}\right)^2\right] \qquad (T \to 0), \tag{39}$$

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being at $T = 0$ completely in agreement with the exact results [28]. In order to find the behavior of $Z(T)$ at arbitrary T, we continue it from the region of $T \to 0$ self–similarly, along the most stable trajectory, with the crossover index s, determined by the condition of the minimum of the multiplier [20-22]

$$m(T, s) = 1 - \frac{1}{6}T^2\frac{1 + s}{s} \ ,$$

from where

$$s(T) = \frac{1}{6}T^2 \left(1 - \frac{T^2}{6}\right)^{-1} \ , \qquad T < \sqrt{6} \ ,$$

$$s \to \infty \ , \qquad T \geq \sqrt{6} \ .$$

This gives the left crossover approximation

$$Z^*(T) = \frac{1}{2}\pi \left(\frac{s(T)}{s(T) + T^2/6}\right)^{s(T)} \ , \qquad T < \sqrt{6} \ , \tag{40}$$

$$Z^*(T) = \frac{1}{2}\pi \exp(-T^2/6) \ , \qquad T \geq \sqrt{6} \ . \tag{41}$$

Formulae (40) and (41) suggest that the spin waves should survive at least up to $T \sim \sqrt{6}$, and become exponentially "soft" above this temperature. Note that in this particular case the left self–similar approximation plausibly reconstructed the function for arbitrary temperatures, even not knowing beforehand the asymptotic behavior at $T \to \infty$.

6.3   Field–dependent part of free energy

It is believed that the magnetic field–dependent part of the free energy of the one–dimensional Heisenberg ferromagnet is independent on spin and scales as $\rho = h/T^2$ (h denotes the magnetic field), with the scaling function independent on the value of spin [32]. For the classical ferromagnet, both low and high field behavior of the field dependent part of the free energy $\delta F(\rho)$ are known [32-35] in the simple form:

$$T^{-2}\delta F(\rho) \sim a\rho^2 + b\rho^4 \ , \qquad a = -\frac{1}{3} \ , \qquad b = \frac{11}{135} \qquad (\rho \ll 1), \tag{42}$$

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$$T^{-2}\delta F(\rho) \sim A\rho + B\rho^{1/2}, \qquad A = -1, \qquad B = 1 \qquad (\rho \gg 1). \tag{43}$$

The left crossover approximation is controlled by the crossover index $s = 1/2$ and crossover time $\tau = -a^3/(2A^2B) = 0.227$, yielding:

$$T^{-2}\delta F^*(\rho,0) = a\rho^2 \left[1 + \left(\frac{a}{A}\right)^2 \rho^2\right]^{-1/2}, \tag{44}$$

while the right crossover approximation is given by

$$T^{-2}\delta F^*(\rho,\infty) = A\rho^2 \left[\rho^{1/2} + \left(\frac{A}{a}\right)^{1/2}\right]^{-2}, \tag{45}$$

with

$$s = 2, \qquad \tau = -2\frac{A}{B}\left(\frac{A}{a}\right)^{1/2} = 3.464.$$

Both expressions (44) and (45) are in good agreement with the known results [32-35].

7   Flexible polymer coil

The calculation of the so–called expansion function $\alpha^2(z)$ of a flexible polymer coil is of long standing interest in polymer science [36-38]. This quantity defines the ratio of the mean square end–to–end distance $< R^2 >$ of the chain to its unperturbed value $< R^2 >_0 \equiv Nl^2$, where N is the number of segments with the length l each, so that Nl is the contour length of the chain,

$$\alpha^2(z) \equiv \frac{< R^2 >}{< R^2 >_0}, \tag{46}$$

as a function of a dimensionless interaction parameter z. The latter is

$$z \equiv \frac{BN}{\pi l^2} \qquad (D = 2) \tag{47}$$

for the two–dimensional case and

$$z = \left(\frac{3}{2\pi}\right)^{3/2} \frac{B\sqrt{N}}{l^3} \qquad (D = 3) \tag{48}$$

for the three–dimensional coil, where B is the effective binary cluster integral for a pair of segments.

When the excluded volume interaction is very weak, a perturbation theory leads [39] to an asymptotic series

$$\alpha^2(z) \simeq 1 + \sum_{n=1} a_n z^n \qquad (z \to 0) , \tag{49}$$

in which the coefficients for the two–dimensional case are

$$a_1 = \frac{1}{2} , \qquad a_2 = -0.121545 , \qquad a_3 = 0.026631 , \qquad a_4 = -0.132236 \qquad (D = 2) ,$$

and for the three–dimensional coil they take the values

$$a_1 = \frac{4}{3} , \qquad a_2 = -2.075385 , \qquad a_3 = 6.296880 , \qquad a_4 = -25.057251 ,$$

$$a_5 = 116.134785 , \qquad a_6 = -594.71663 \qquad (D = 3) .$$

The asymptotic result for the strong coupling limit [40] is

$$\alpha^2(z) \simeq A_1 z^\beta + A_2 z^\gamma \qquad (z \to \infty) . \tag{50}$$

Using our method of self–similar interpolation, we obtain from (49) and (50)

$$\alpha_*^2(z) = \left(1 + A_1^{1/\beta} z\right)^\beta \tag{51}$$

in the first approximation. The second approximation gives

$$\alpha_*^2(z) = \left[(1 + C_1 z)^{2-\beta+\gamma} + C_2 z^2\right]^{\beta/2} , \tag{52}$$

where

$$C_1 = \left(\frac{2A_2}{\beta A_1^{1-2/\beta}}\right)^{1/(2-\beta+\gamma)} , \qquad C_2 = A_1^{2/\beta} .$$

These formulae can serve for both the two– as well as for three–dimensional coils. We shall concentrate on the latter case for which accurate numerical data for $\alpha^2(z)$ are available [40] in the whole range of $z \in [0, \infty)$. Then in the strong coupling limit (50), one has

$$A_1 = 1.5310 , \qquad A_2 = 0.1843 , \qquad \beta = 0.3544 , \qquad \gamma = -0.5756 \qquad (D = 3) . \tag{53}$$

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The coefficients in (52) become

$$C_1 = 6.5866 \;, \qquad C_2 = 11.0631 \;, \qquad 2 - \beta + \gamma = 1.07 \;.$$

In this way, from (52) we obtain

$$\alpha_*^2(z) = \left[(1 + 6.5866z)^{1.07} + 11.0631z^2\right]^{0.1772} \;. \tag{54}$$

The self–similar approximation (54) is accurate, within 0.4% of error, in the full range $z \geq 0$, as compared to numerical calculations [40]. This formula (54) practically coincides with the phenomenological extrapolation expression

$$\alpha_{MN}^2(z) = \left(1 + 7.524z + 11.06z^2\right)^{0.1772} \;, \tag{55}$$

obtained by Muthukumar and Nickel [40] by means of a fit to numerical data.

In conclusion, we have developed the *method of self–similar interpolation* for deriving explicit interpolation formulae for difficult crossover problems of statistical mechanics. This method, as is illustrated by several examples, is general, simple, and accurate.

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